Supplementary Material

1. Potential energy of the reactant/transition/product state from Jaguar calculations.

These are results from the DFT calculations without ZPE (zero-point energy) and solvation corrections. They describe the reactant and product energies when all of the species in the transition state are nearby. The reactant and product energies described in the main text show the energies when the molecules that take part in the reactions are infinitely far apart including ZPE and solvation corrections.

Potential energy surface to the reaction in

Fig. 2:

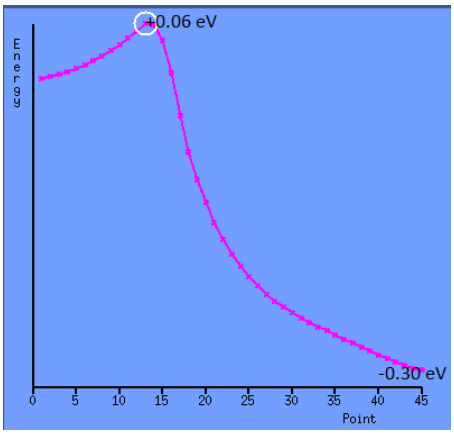


Fig. 3C:

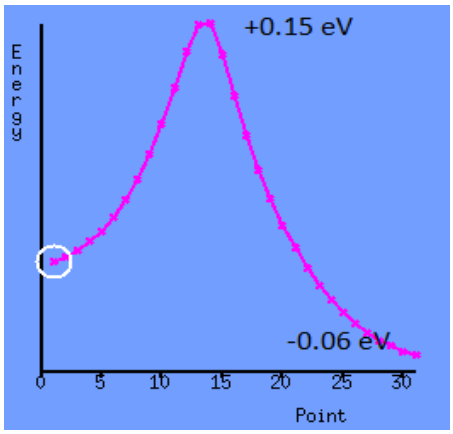


Fig. 3D

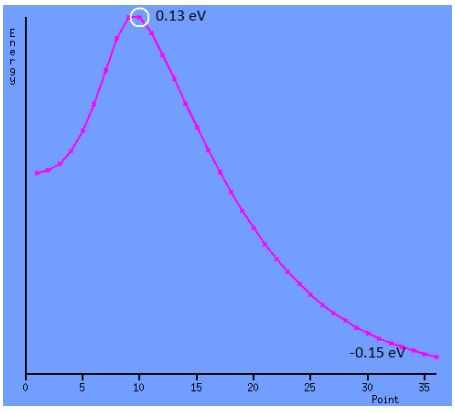


Fig. 4A

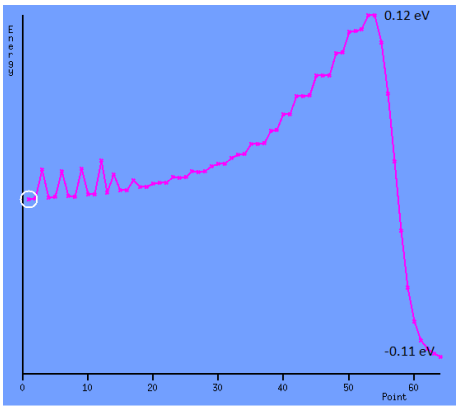


Fig. 4B:

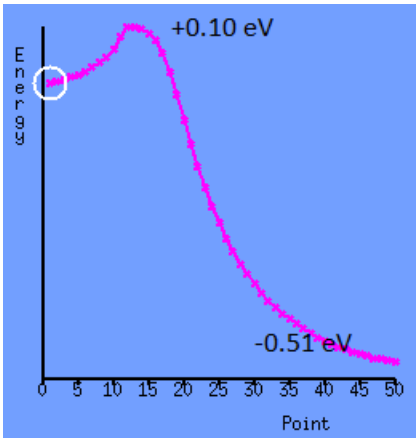


Fig. 5Bi:

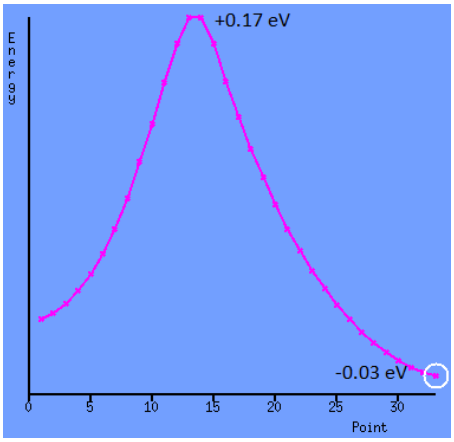


Fig. 5Ci:

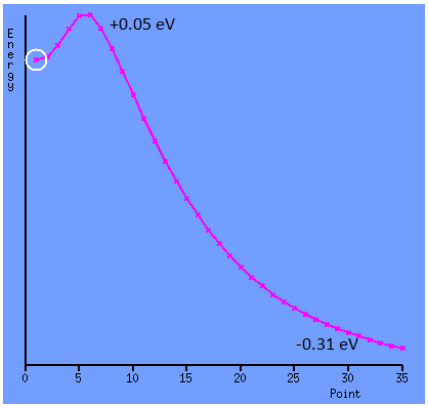


Fig. 5Bii:

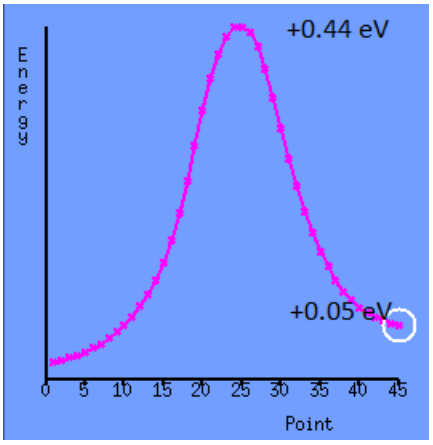


Fig. 5Cii:

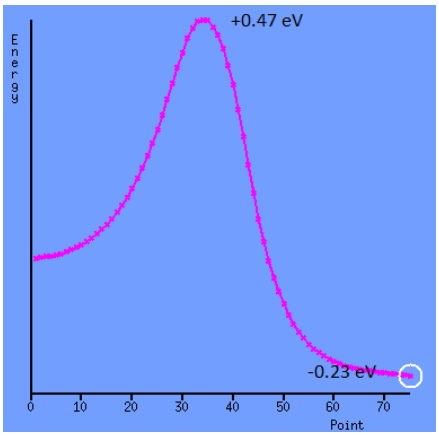


Fig 6B

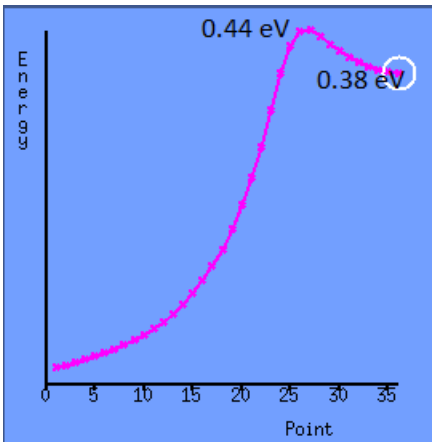


Fig. 6C

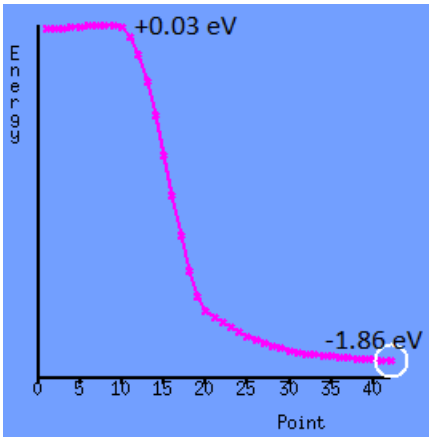


Fig. 7B

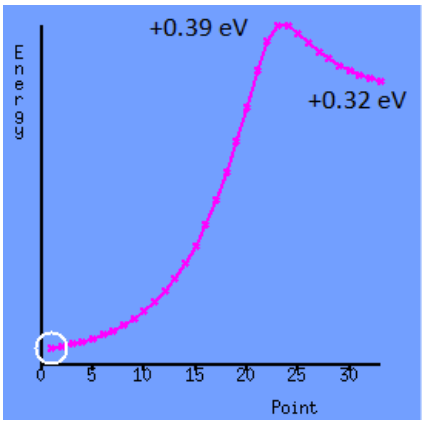


Fig. 7C

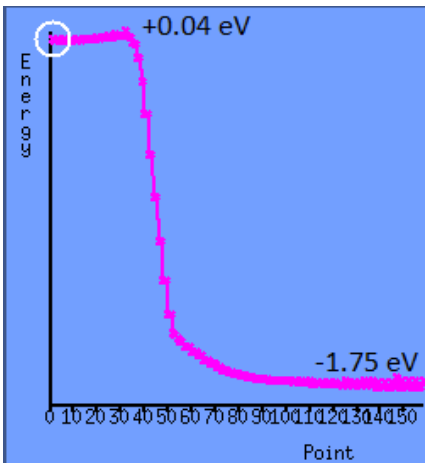


Fig. 8A:

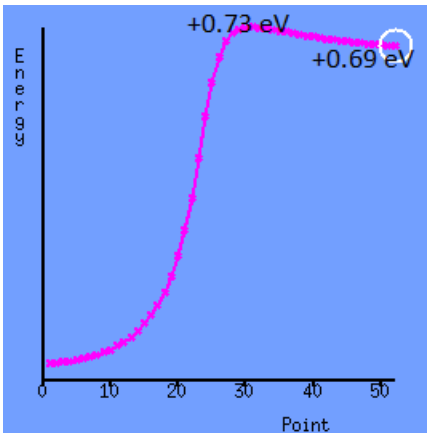


Fig. 8B:

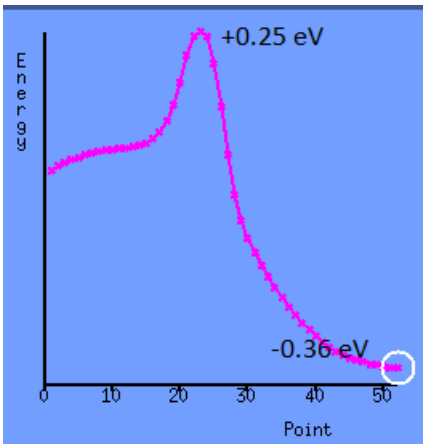


Fig. 8C:

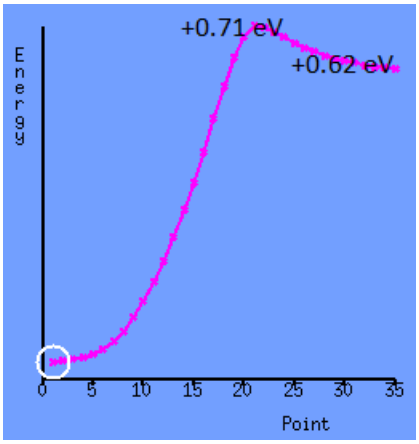


Fig. 9A:

Fig. 9B:

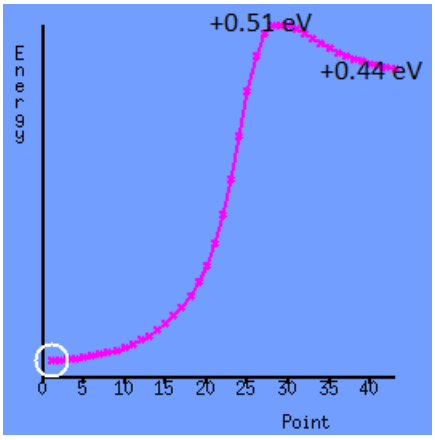


Fig. 11A:

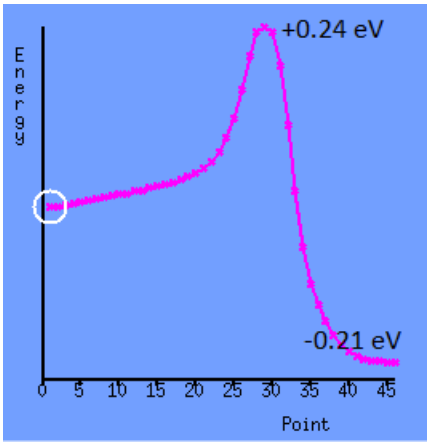


Fig. 11B:

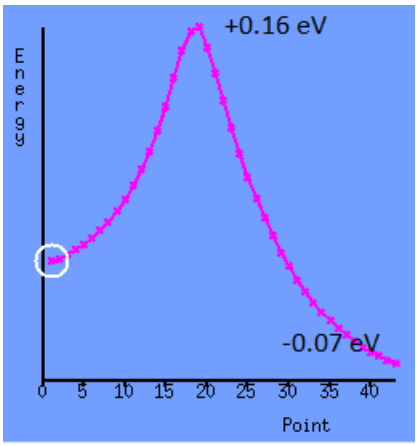


Fig. 12B:

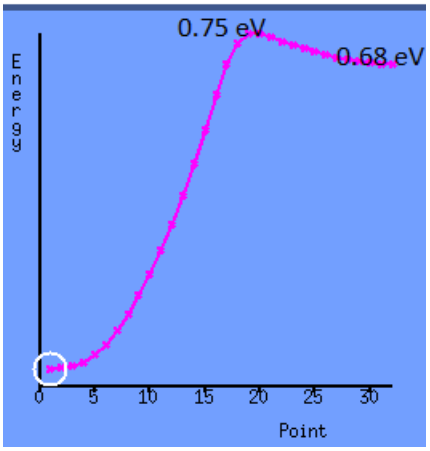
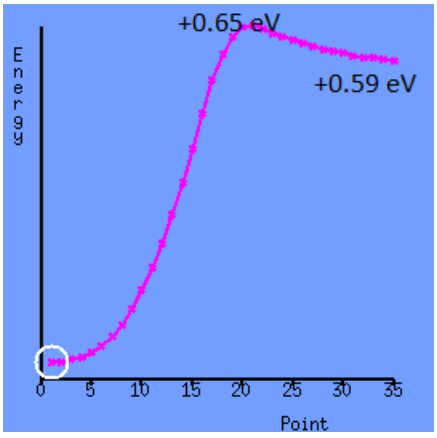


Fig. 13A:



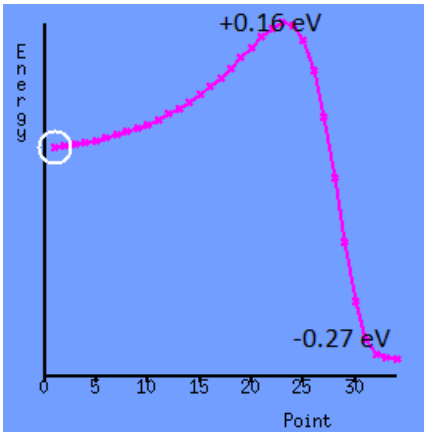
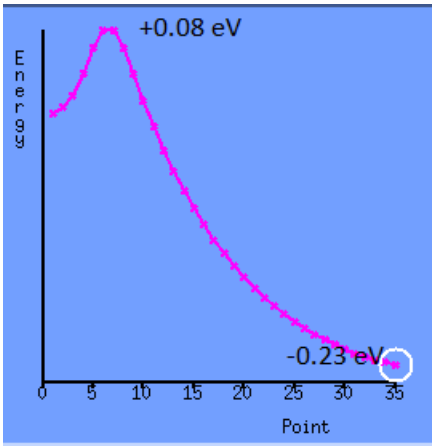
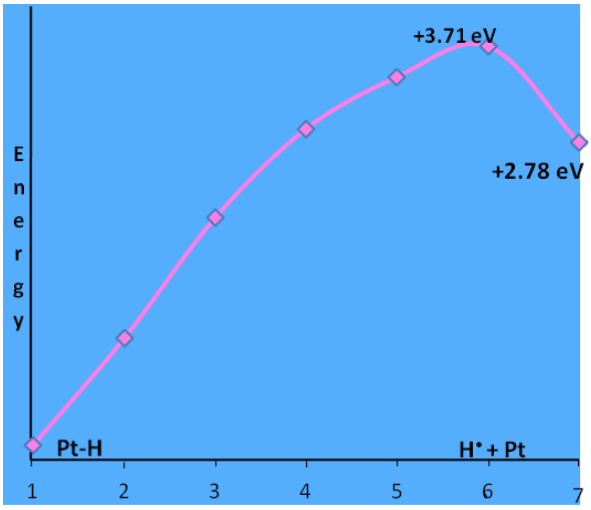


Fig. 13B:



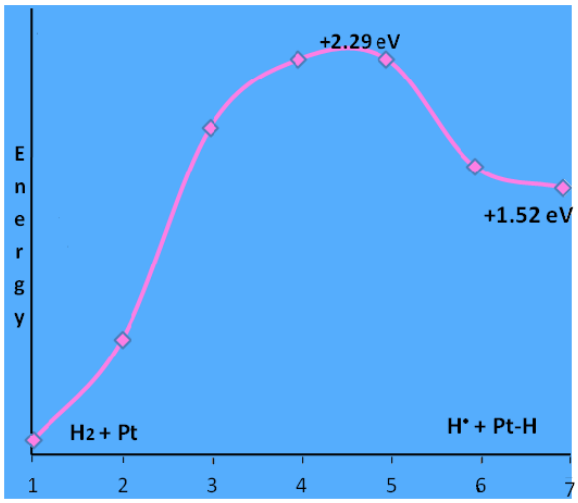
2. NEB data for the formation of H radical from H_{ad} or H_2 on a Pt (111) surface shown in Figure 10A and 10B.

To Fig. 10A:



The barrier for the removal of H$^{\bullet}$ from the Pt (111) surface.

Fig. 10B:



The transition state and barrier of the reaction Pt (111) + H_2 → Pt(111)–H + H$^{\bullet}$.